Supporting information

Batch and Fixed-Bed Adsorption Behavior on Porous Boehmite with High Percentage of Exposed (020) Facet and Surface Area towards Congo Red

Zijia Li,[a] Li He,[a] Weiliang Tian,[b] Renyao Huang,[c] Xingpeng Wang,[a] Dianqing Li,[a] Pinggui Tang,[a] and Yongjun Feng[a,b]**

[a] State Key Laboratory of Chemical Resource Engineering, College of Chemistry, Beijing University of Chemical Technology, No. 15 Beisanhuan East Road, Beijing, 100029, China.

[b] Key Laboratory of Chemical Engineering in South Xinjiang, College of Life Science, Tarim University, Alar 843300, P. R. China

[c] Beijing OriginWater Membrane Technology Co., Ltd., No. 4 Leyuan South Second Street, Yanxi Economic Area, Huairou District, Beijing, 100000, China

Corresponding Author: [a] E-mail: yjfeng@mail.buct.edu.cn; Fax: +86-10-64448071; Tel: +86-10-64448071; [b*] E-mail: twllong@126.com

Number of pages: 9 **Number of figures: 9** **Number of tables: 3**

Section S1. Supporting Information of Boehmite Powder

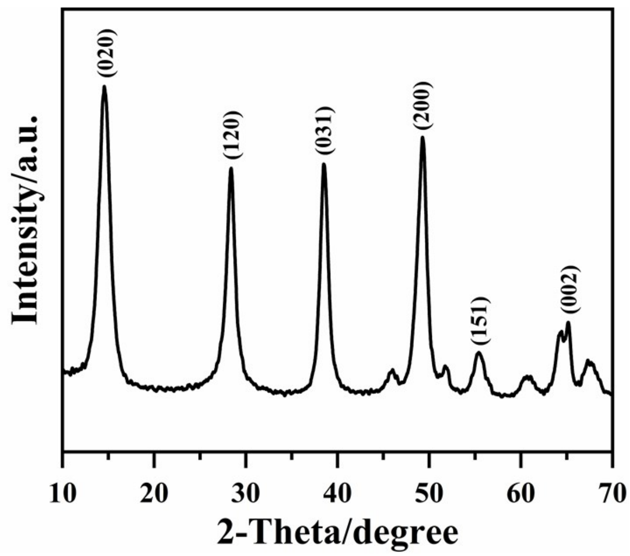

Fig. S1 Powder X-ray diffraction (PXRD) pattern of reference sample obtained by twice hydrothermal treatment.

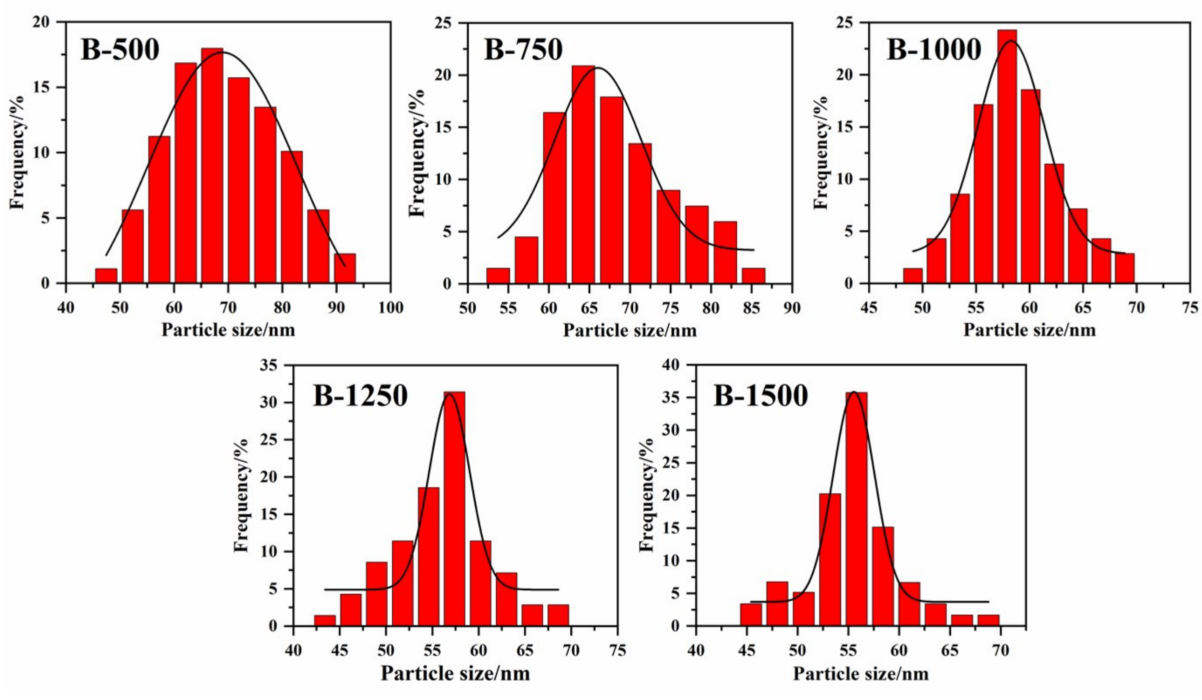

Fig. S2 Particle size distribution of the obtained boehmite at the different speeds from 500 to 1500 rpm.

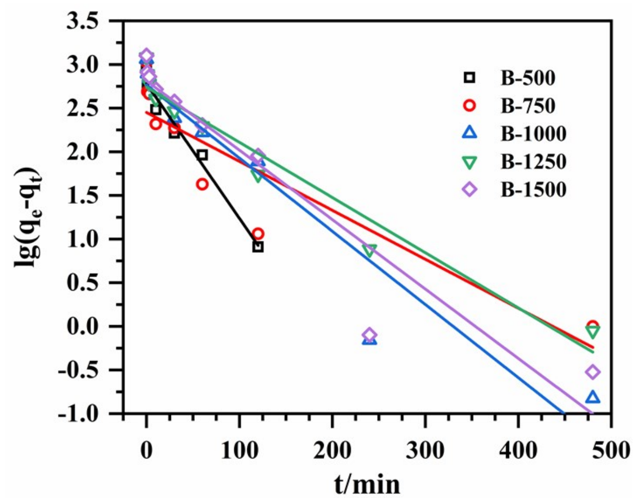

Fig. S3 The linear fitting of the pseudo-first-order kinetics for CR by the different boehmite samples from 500 rpm to 1500 rpm.

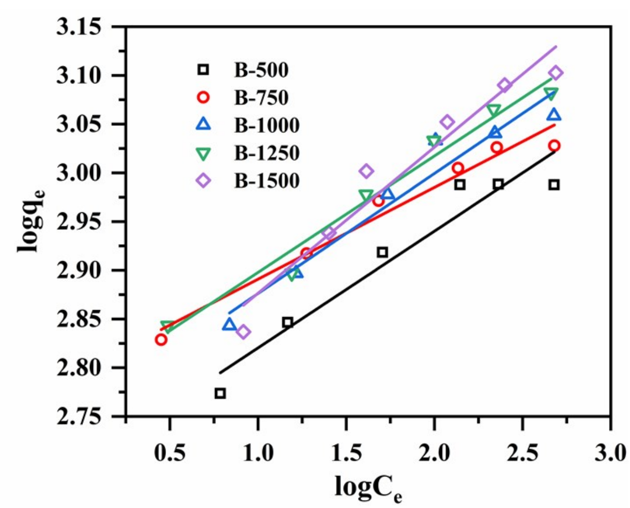

Fig. S4 The linear fitting of the Freundlich isotherm for CR by the different boehmite samples from 500 rpm to 1500 rpm.

Table S1 Parameters of linear fitted by the pseudo-first-order and pseudo-second-order kinetics models for CR adsorption

Samples	$q_{e,exp}$ (mg g^{-1})	Pseudo-first-order model			Pseudo-second-order model		
		$q_{e,cal}$(mg g^{-1})	k_1 (min^{-1})	R^2	$q_{e,cal}$ (mg g^{-1})	k_2 (mg $(gmin)^{-1}$)	R^2
B-500	933.90	16.15	0.0356	0.972	943.40	0.00027	0.9996
B-750	1064.0	11.60	0.0129	0.824	1068.8	0.00036	0.9999
B-1000	1153.6	15.89	0.0193	0.926	1139.0	0.00014	0.9998
B-1250	1212.4	15.50	0.0146	0.955	1224.0	0.00013	0.9998
B-1500	1266.8	16.66	0.0183	0.907	1282.1	0.00011	0.9997

Table S2 Parameters of linear fitted by Langmuir and Freundlich models for CR adsorption

Samples	Langmuir isotherm			Freundlich isotherm		
	q_{max}(mg g^{-1})	K_L(L mg^{-1})	R^2	K_F(mg g^{-1})(L mg^{-1})$^{1/n}$	n	R^2
B-500	990.10	0.1906	0.9998	14.89	8.354	0.9323
B-750	1077.6	0.1871	0.9998	16.39	10.62	0.9692
B-1000	1160.1	0.1181	0.9997	15.68	8.117	0.9474
B-1250	1227.0	0.1086	0.9994	16.09	8.368	0.9746
B-1500	1293.7	0.0831	0.9997	15.28	6.676	0.9459

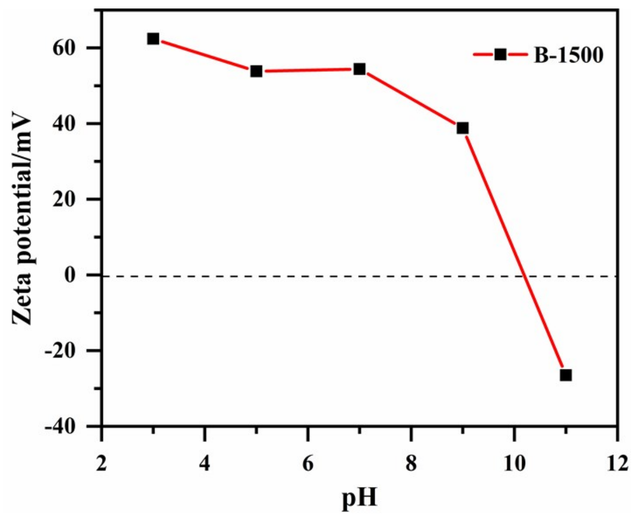

Fig. S5 Zeta potential of B-1500 at different solution pH values.

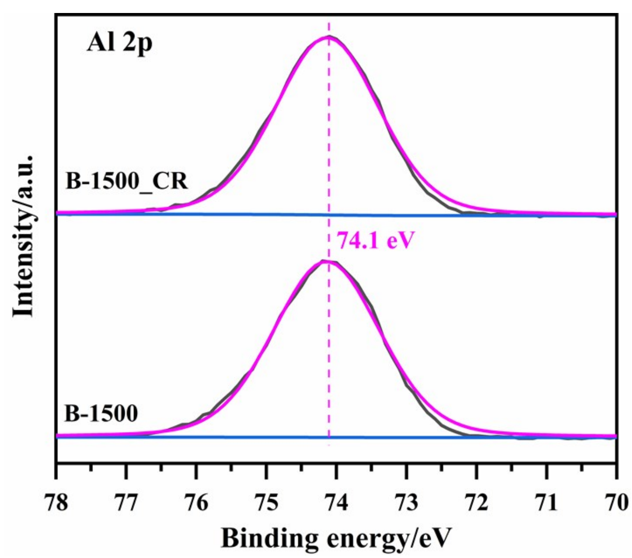

Fig. S6 XPS spectra of Al 2p for B-1500 before and after CR adsorption in aqueous solution.

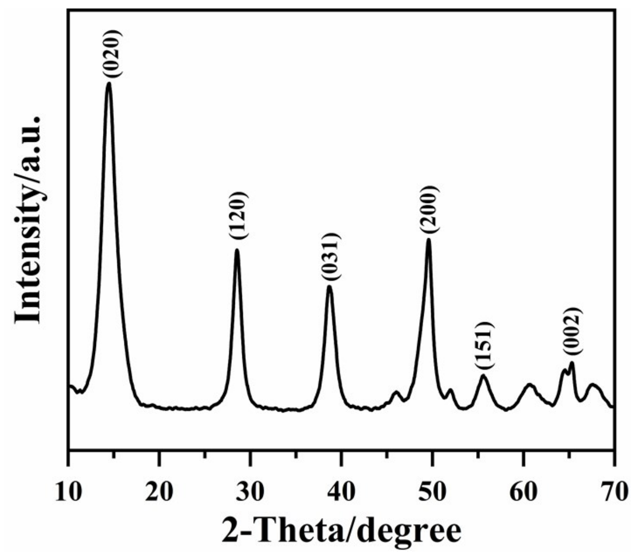

Fig. S7 Powder X-ray diffraction (PXRD) pattern of B-1500s prepared in a 5 L hydrothermal reactor.

Table S3 Crystal facet parameters of B-1500s

Samples	D_{020} (nm)	D_{200} (nm)	D_{002} (nm)	Percentage of exposed (020) facet (%)
B-1500s	8.23	13.56	37.32	54.73

Section S2. Supporting Information of Boehmite Pellet

Fig. S8 shows XRD pattern of the composite. Here one observes that the alginate-boehmite composite still remains the crystal structure of boehmite with the percentage of exposed (020) of 53.69%, which is comparable with that of 54.73% for B-1500s before molding. Therefore, it is stable under the investigated conditions.

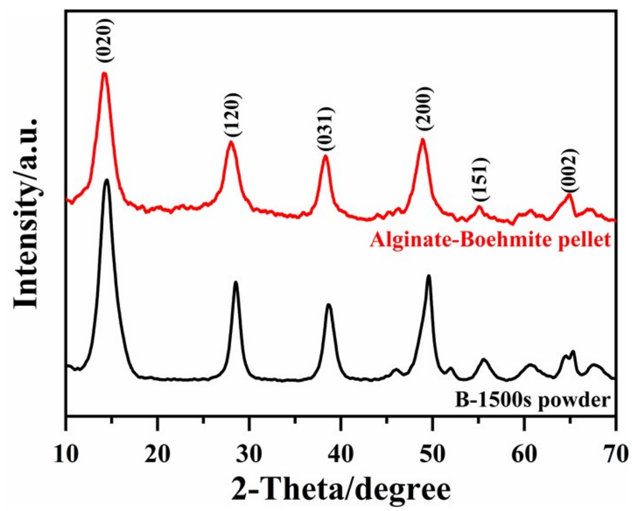

Fig. S8 Powder X-ray diffraction (PXRD) pattern of B-1500s powder and boehmite pellets prepared by alginate-assisted molding route.

In this work, one observes that the decrease of adsorption capacity after molding, and the percentage of performance degradation was measured by adsorption experiment. Adsorption for CR on boehmite pellets were performed in 250 mL Erlenmeyer flask that contained pellets with a net content of 10 mg boehmite and 50 mL CR solution of 200 mg L^{-1}, as well as the adsorption performance of B-1500s was tested by the same method. Afterwards, the system was shaken in a shaker at 25℃ for 12 h. After the adsorption was completed, separating the pellets and solution, and then the CR concentration in the solution was measured. As shown in Fig. S9, the removal efficiency of B-1500s and the corresponding pellets under the same measuring conditions are 98.6% and 70.4%, respectively. The removal efficiency of pellets decreased ca. 29% compared with the B-1500s. The phenomenon is attributed to a decrease in the percentage of exposed the adsorption sites and the specific surface area. During the molding process, alginate covers the boehmite to the certain extent, which leads to a reduction in the adsorption sites and reduces the contact area between the solution and the active ingredient. Besides, the phenomenon of adsorption performance degradation after molding has been found in other materials,[1-3] but the percentages of performance degradation based on these materials are more than 35%. These results suggest that boehmite pellets in this work have advantage after molding and exhibit promising practical applications for removal CR from water.

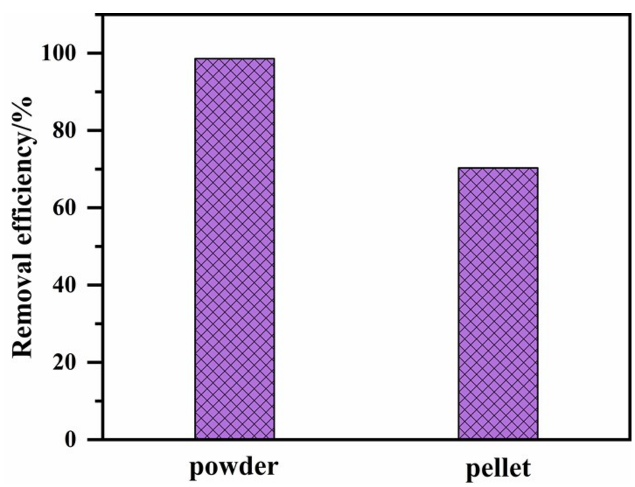

Fig. S9 The removal efficiency of B-1500s powder and the corresponding pellets for CR solution.

References

1. A. Charkhi, M. Kazemeini, S. J. Ahmadi and H. Kazemian, Fabrication of granulated NaY zeolite nanoparticles using a new method and study the adsorption properties, *Powder Technol.*, 2012, **231**, 1-6.
2. A. Charkhi, M. Kazemeini, S. J. Ahmadi and S. Ammari Allahyari, Effect of bentonite binder on adsorption and cation exchange properties of granulated nano NaY zeolite, *Adv. Mater. Res.*, 2011, **335-336**, 423-428.
3. R. N. Putra and Y. H. Lee, Entrapment of micro-sized zeolites in porous hydrogels: Strategy to overcome drawbacks of zeolite particles and beads for adsorption of ammonium ions, *Sep. Purif. Technol.*, 2020, **237**.